MS Imaging in plant metabolomics: a data analysis perspective

Pietro Franceschi, Yonghui Dong, Fulvio Mattivi, Urska Vrhovsek, Ron Wehrens

Research and Innovation Centre – Fondazione Edmund Mach

Via Mach 1, 38010 San Michele all'Adige (TN) – Italy

E-mail: pietro.franceschi@fmach.it

The visualization of the spatial distribution of metabolites and bioactive compounds in tissues can improve our understanding of biological processes occurring in plants, with important technological, nutritional and economical implications.

High resolution MS based techniques represent an excellent tool to study the distribution of small molecules in tissue, but in view of possible high-throughput applications it is also necessary to develop innovative bioinformatic tools for data analysis and interpretation.

Among the diverse critical aspects, metabolite identification is particularly relevant because it is a prerequisite to every biological interpretation. However, it cannot only be performed relying on (high resolution) mass to-charge ratios. In a recent publication (Franceschi, 2012) we propose to use co-localization of characteristic molecular fragments to visualize the asymmetric distribution of relevant metabolites in Golden Delicious apples.

In a wider perspective, data segmentation and signal clustering are other promising research fields ifor automatic data mining of MS imaging datasets.

In this contribution preliminary results of the analysis of several DESI and MALDI imaging datasets will be presented and discussed.

References

Franceschi, P., Dong, Y., Vrhovsek, U., Mattivi, F. 2012. "Combining intensity correlation analysis and MALDI imaging to study the distribution of flavonols and dihydrochalcones in Golden Delicious apples", J. Exp. Bot. 63(3):1123-1133.